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## REPORT

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CD NO.

DATE OF INFORMATION 1950

DATE DIST. 19 Oct 1950

50X1-HUM

NO. OF PAGES 7

SUPPLEMENT TO  
REPORT NO.

REPORT NO.

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Izvestiya Akademii Nauk SSSR, Otdeleniye Khimicheskikh Nauk, No 4,  
1950, pp 438-44.

## USSR CHEMISTS' ATTACK ON THE RESONANCE THEORY OF CHEMICAL STRUCTURE

A. P. Meshcheryakov

In the following digest, Ya. K. Syrkin and M. Ye. Dyatkina bear the brunt of an attack by USSR chemists on the resonance theory of chemical structure. Among those criticized are A. N. Nesmeyanov and M. I. Kabachnik. The question of revision of organic chemistry textbooks is raised. The discussion will be continued in future issues of chemical periodicals.

On 2, 3, and 7 February 1950, an expanded meeting of the Scientific Council of the Institute of Organic Chemistry of the Academy of Sciences USSR, took place under the chairmanship of A. N. Nesmeyanov, the institute's director. The attendance was 54, 88, and 114, respectively, on the 3 days in question.

The meeting concentrated on a discussion of the report "On the Contemporary State of the Theory of Chemical Structure" presented by Professor D. N. Kursanov in the name of a group of collaborators of the institute. In this report, Kursanov pointed out the practical value and vital significance of A. M. Butlerov's materialistic theory of chemical structure as opposed to the resonance theory, which is based on an essentially idealistic concept. The latter theory has been persistently advocated in the USSR by Ya. K. Syrkin, M. A. Dyatkina, A. I. Kipriyanov, and several other chemists.

Many Russian investigators in the field of chemistry have begun to accept the harmful viewpoint that all explanations of chemical reactions must be brought into agreement with the "contemporary" resonance theory, purely as a matter of convenience. At the same time, the theory developed by Butlerov's school was neglected as being allegedly based on primitive early-twentieth-century electrostatic concepts. Such groveling before Western bourgeois science, combined with neglect of the achievements of Russian chemists, must have had a deleterious effect on the development of Soviet organic chemistry. Reflected against this background, Kursanov's report could not have failed to arouse considerable attention.

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[This is Meshcheryakov's statement. It is somewhat difficult to determine whether the preceding text represents a report on Kursanov's paper or an expression of Meshcheryakov's own views.]

Kursanov stated that, according to Butlerov, only one formula is possible for any one chemical compound and that this formula expresses all properties of the compound. Kursanov further pointed out that the crisis of bourgeois science had influenced the theory of organic chemistry developed by bourgeois scientists, so that harmful theories holding back the progress of science resulted. He cited numerous examples demonstrating that American scientists, L. Pauling, G. W. Wheeland, and others, have merely perverted the real meaning of Butlerov's theory. Foreign scientists, according to Kursanov, were guided by Mach's idealistic philosophy in developing the theory of resonance.

Kursanov particularly condemned the uncritical attitude exhibited by Ya. K. Syrkin and M. E. Dyatkina toward Pauling's resonance theory in their book The Chemical Bond and the Structure of Molecules. On the other hand, he praised the criticism contained in papers published by G. V. Chelintsev and Ufimtsev. He further reviewed Chelintsev's book Outline of the Theory of Organic Chemistry and stated that the author's attempt to explain all phenomena in organic chemistry by orbital and contact bond effects does not lead to entirely convincing results.

Tatayevskiy commented on Kursanov's report by agreeing that the resonance theory is essentially based on Mach's principle of describing phenomena in the most convenient manner. He further stated that the resonance theory, in attempting to apply the terminology and methods of quantum chemistry, actually distorts the terminology and the physical meaning of values which enter into quantum-chemical calculations. According to Tatayevskiy, the theory of resonance holds that the function of the basic state can be expressed by a linear combination of functions, each of which determines some particular state of the system. This assumption results in a fundamentally wrong interpretation of quantum-mechanical relationships, he stated. The underlying invalid interpretation of the physical meaning of individual wave functions being added has been made by Pauling, Wheeland, Syrkin, Dyatkina, and Bocharov, he continued. Tatayevskiy went on to say that this is a fundamental error of the resonance theory due to a misinterpretation of the physical meaning expressed by the linear variant of the variation method, and actually has no bearing on the resonance theory itself. The inaccurate interpretation is due to attempts to substitute speculative schemes and concepts for actuality.

G. V. Chelintsev stated that the resonance-mesomerism theory has been advertised extensively and accepted uncritically. Furthermore, he stated, it originated in Anglo-Saxon countries and is definitely based on Mach's method.

I. L. Knunyants, Corresponding Member of the Academy of Sciences USSR, said that Cooper formulas of molecular structure are based exclusively on the corpuscular function of the electron. If we consider the wave function in addition to the corpuscular function, we will undoubtedly return to Markovnikov's and Butlerov's theory of structure, Knunyants concluded.

M. E. Dyatkina emphasized that mathematical methods as applied in the determination of possible valency structures of multielectron systems do not permit any conclusion in regard to the actual existence of some particular structure. She admitted that, from the qualitative viewpoint, errors which have led to an incorrect understanding of the theory may have been committed.

M. I. Kabachnik, after pointing out that there is no such quantum-mechanical phenomenon as the resonance of structures, stated that the assumption of any such phenomenon did not simply originate due to faulty language. He said that there is a wrong idea there rather than incorrect use of the language, and Pauling has devoted a whole chapter to that idea. Kabachnik went on to say that quantum-mechanical calculations are justified, but one should not refer to the results of such

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calculations as the resonance theory, because otherwise the whole of quantum mechanics will enter into the resonance theory. Thereupon, Kabachnik pointed out the lack of criticism and objectivity exhibited in his own article on orientation in the benzene ring published in *Uspekhi Khimii* during 1948. In conclusion, Kabachnik praised Chelintsev for criticizing the resonance theory, but demonstrated the shortcomings of Chelintsev's own theory on the examples of the structures of benzene and nitrobenzene.

A. P. Meshcheryakov stated that, from the practical viewpoint, the theory of resonance sets back chemical research. The activity of proponents of that theory (Syrkin, Dyatkina, Kiprianov, Vol'kenshteyn, and others) should be judged accordingly, he said. The resonance theory is based on an idealistic approach and the tendency of the people who advocated it was to disregard or at least distort the achievements of Russian chemists, he concluded.

B. M. Mikhaylov, M. G. Gonikberg, and D. A. Bochvar then expressed their agreement with Kursanov's essential thesis, and B. M. Dubinin raised a question in regard to the meaning of "contact bond," which, according to Chelintsev, may be either heteropolar or homopolar.

R. Kh. Freydlina, in her talk, brought out, among other things, that the theorists of resonance, Pauling and Wheland, are representatives of an idealistic school which is fashionable in the USA.

Professor V. A. Izmail'skiy said that attempts made 37 years ago to formulate relationships explaining the coloration of organic compounds led him to the concept which he originally called "mesostructure" or "mesostate" and which later became known as mesomerism. In defining mesomerism, Izmail'skiy referred to electron shifts which cause formation of structures differing from the classical. The classical formula, in Izmail'skiy's opinion, expresses only an idealized state arrived at by a sort of averaging or summation. Izmail'skiy agreed that the characterization of the status of the structural theory given by Kursanov is correct and stated that the criticism of the resonance theory advanced by the latter is compatible with a quantum-mechanical treatment of mesomerism. He concluded by emphasizing that further development of the theory of structure in the sense of Butlerov's conception of mutual interaction and interdependence of individual atoms constituting a molecule will expedite industrial progress.

N. D. Sokolov remarked that results of proximate quantum-mechanical calculations in the field of theoretical chemistry cannot be regarded as achievements of the theory of resonance. Sokolov went on to say that one can only condemn a too literal interpretation of these results and methods in the sense of the resonance theory.

Ya. K. Syrkin admitted that he and his collaborator, M. E. Dyatkina, have made a number of errors in their book and that through sheer oversight they have also introduced some inept formulations. He further stated that, in writing the book, insufficient attention was given to ideological aspects, although ideology plays an important and significant role in physics and, apparently, also in chemistry. Syrkin stated that a discussion involving the principles of quantum mechanics is now being carried on abroad. In the course of this discussion he said, some physicists have reached conclusions which are entirely unacceptable. Thus, Heisenberg in the paper "Electrons and Terminism" develops ideas which may lead to the assumption that the electron possesses a free will. The controversy taking place abroad has also been reflected in the USSR, Syrkin continued. USSR theoreticians in the field of quantum mechanics (Blokhintsev, Fok, et al.) are now improving their inexact formulations and introducing more precision into their fundamental assumptions.

Syrkin stated that he assumes full responsibility for the fact that a certain amount of negligent writing has been included in his book. He further recognizes that he and Dyatkina have aggravated the errors of Pauling's method of

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transition structures. Syrkin went on to say that instead of bringing the function itself into agreement with the structure, they brought into agreement with the structure the square of the modulus of the function. The transition structures obtained in this manner were inaccurate, he said, because he and Dyatkina arbitrarily divided the electron cloud into three parts and assumed Heilster's transitional charge cloud to be the structure. Furthermore, Syrkin admitted the cardinal error of underestimating Butlerov. In conclusion, he stated that Kursanov's criticism is justified and that people who advocate the resonance theory have not been criticized enough in Kursanov's report.

Academician A. N. Nesmeyanov, in his address, first illustrated the concept of mesomerism on the examples of the  $\text{CO}_2$  ion and the acid amides. He pointed out that from the standpoint of quantum mechanics a certain distribution of electron density corresponds to a genuine acid amide, and that this distribution can be expressed by a wave function  $\psi$ . Furthermore,  $\psi$  can be expanded into a series:

$$\psi = \psi_1 + b\psi_2$$

Keeping in mind that this is a purely mathematical manipulation Nesmeyanov continued, one must first ask the question as to whether there is a correspondence between the members of this series and the idealized structures which do not occur in nature, but represent abstract limits. Quantum physicists answer that such correspondence is possible in a rough approximation. It is another matter to decide just how accurate this representation is. Nesmeyanov went on to say that everybody understands resonance according to his own lights, and asked whether an acetamide which is expressed by two structural formulas actually exists in nature.

There is definitely no such acetamide in nature, Nesmeyanov continued, but a compound in which the two structures have been averaged out. However, Nesmeyanov stated, in assuming extreme structures we do not deal with figments of our imagination. Structures corresponding to the idealized, extreme cases for acetamide actually exist in acetaldehyde and ketones on the one hand and compounds of the type of ammonia and amines on the other hand, he said. All this is quite real and actual: idealism begins when someone starts to imagine that there is an interaction between mathematical formulas and that it is this interaction which determines the behavior of the substance. Unfortunately, he stated, the description found in some translated and original books is so vivid that the readers may actually suspect the author of believing that this interaction actually occurs. Nesmeyanov concluded by saying that in Kursanov's report there was very little criticism of actual errors committed by workers of the Institute of Organic Chemistry and that he, Nesmeyanov, has been guilty of an uncritical attitude toward Pauling and the resonance theory in general.

The balance of Nesmeyanov's address was devoted to a detailed discussion of Chelintsev's new theory of structure and a critical review of the concepts of the orbital and contact bond.

After Nesmeyanov's address, Ye. D. Kaverzneva declared in the name of the group which had participated in the preparation of Kursanov's report that Syrkin's talk admitting the justice of criticism directed against his and Dyatkina's book has not demonstrated a sufficiently critical attitude on Syrkin's part.

A. D. Petrov, Corresponding Member of the Academy of Sciences USSR, emphasized the necessity of developing Butlerov's theory further and stated that Ya. K. Syrkin must be regarded as a proponent of harmful idealistic concepts. Petrov went on to say that substances must not be regarded abstractly, as in the resonance theory, but studied under actual conditions, taking into consideration the surrounding medium. What is needed, Petrov said, is further study of the direction in which reactions proceed and work on the synthesis of new compounds.

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I. N. Nazarov, Corresponding Member of the Academy of Sciences USSR, stated that the resonance theory has resulted from the impact of idealistic physical theories on chemistry and consequently must be rejected as reactionary. Nazarov went on to say that in resonance there is an element of the speculative, of the arbitrary behavior of chemical substances in reactions. This is something against which he and his group must categorically protest, he said. Nazarov further remarked that mistakes made by R. Kh. Freydlina and A. N. Nesmayanov have not been adequately shown in Kursanov's report, and that Freydlina's talk has demonstrated a lack of self-criticism.

N. I. Shuykin remarked in his address that Kursanov's report has presented a matter-of-fact criticism directed against the harmful idealistic concept on which the resonance theory is based. Furthermore, he continued, a somewhat inadequate attempt has been made in this report to lead the development of theoretical organic chemistry into a different channel under the guiding principle of mesomerism rather than resonance and in accordance with the ideas of Butlerov and Markovnikov. Kursanov's report, Shuykin added, incorrectly states that it does not make much difference how molecules are represented. There should be one method rather than any number of arbitrary methods for representing molecules.

Professor P. P. Shorygin brought out that many Soviet chemists were influenced by the tremendous build-up given to the resonance theory and were misled as far as its scientific value is concerned. The propaganda involved here, Shorygin said, has done a lot of harm to the development of national chemistry, because the thinking of investigators was directed into wrong channels. In the theory of resonance, Shorygin said, the understandable is explained by the incomprehensible. It is unfortunate that USSR scientists like Syrkin and Dyatkina have surpassed Western scientists in their adherence to the concept of resonance as an actually occurring physical phenomenon.

O. A. Reutov added that the resonance theory has been the keystone of Syrkin's theoretical credo. He stated that, together with Pauling, he regards resonance as a physical phenomenon. Under the circumstances, Reutov added, it would be useless to expect any criticism of Pauling's views from Syrkin. Discussing the circumstances which led to a penetration of a speculative and idealistic theory into the USSR, Reutov stated that (1) there has been an uncritical attitude toward the theory advanced by foreign scientists and Syrkin is the man who is primarily responsible for this, and (2) theoretical developments were neglected by some prominent USSR chemists who have forgotten the tradition of Russian chemistry, which always emphasized theory.

V. K. Matveyev, Candidate of Chemical Sciences (Institute of Organic Chemistry, Academy of Sciences USSR), remarked that V. A. Izmail'skiy rather than A. Ye. Poray-Koshits must be regarded as the originator of the concept of mesomerism.

I. V. Obreimov, Corresponding Member of the Academy of Sciences USSR, stated that the quantum theory has contributed a lot to chemistry, including an explanation of the valency bond, which from the viewpoint of the quantum theory is quite correctly represented by the conventional dash. Obreimov then criticized resonance theory, which formulates all possible structures (about 97 in the case of anthracene), but does not formulate the correct structure. The adherents of the resonance theory, Obreimov stated, do not ask whether the lattices are degenerate or not, but blithely formulate a linear combination of all functions.

Professor B. M. Berkengeym, editor of *Uspekhi Khimii*, admitted that the editorial board of that journal mistakenly stated in a footnote to M. I. Kabachnik's article that everything which is in accordance with the resonance theory may be retained as a working hypothesis by chemists.

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M. I. Batuyev stated in a very enlightening address that Kursanov was not quite consistent as far as criticism of C. K. Ingold's theory of mesomerism is concerned. The idealism contained in Ingold's theory was consciously smuggled in, according to Batuyev, in order to retain the concept of mesomerism. There is no difference between the theory of mesomerism and the theory of resonance, according to Batuyev.

V. I. Ivanov stated that the harmful theory of resonance has been propagandized within the walls of the Institute of Organic Chemistry for a long time. In the course of discussing the Machist methodology inherent in the theory propounded by Pauling, Wheland, and others, Ivanov remarked that it could be seen from Syrkin's and Dyatkina's addresses that these scientists were still defending the Machist and idealistic views of Pauling and Wheland. Syrkin and Dyatkina, Ivanov said, do not realize that they have committed methodological and political errors. They concentrated on propagandizing Mechism and proving its premises, while slighting national science. Thus, according to Ivanov, Syrkin and Dyatkina do not mention pre-Revolutionary and Soviet authors in their monograph, but mention less prominent foreign authors.

V. V. Korshak, T. I. Temnikova, Ye. N. Prilezhayeva, and several others also took part in the debate.

In concluding, Kursanov pointed out the significance of the debate and the necessity of developing a theory of structure and reactivity which is anchored to practical applications. According to Kursanov, the present discussion has shown that the concept of mesomerism has been expanded in such a manner that it no longer corresponds to Izmail'skiy's and Ingold's mesomerism. Mesomerism will have to be more precisely defined, in Kursanov's opinion.

On conclusion of the discussion, the following resolution was carried:

1. Kursanov's report, "On the Contemporary Status of the Theory of Chemical Structure," has correctly evaluated the contributions made by Butlerov, Markovnikov, and other Russian chemists to the theory of chemical structure, which when correctly formulated is indissolubly tied up with practical applications and leads toward further progress in the field of organic chemistry.
2. Kursanov's report justly criticizes the concepts developed by bourgeois scientists (Pauling and Wheland). The idealistic character of the resonance theory has been shown in this report; furthermore, it has been shown that the meaning of Butlerov's theory has been distorted by bourgeois scientists, who gave insufficient credit to Butlerov.
3. The Scientific Council's discussion of the report has shown that a section of Soviet chemists has accepted and used the resonance theory without applying due criticism. This is reflected in monographs written by Ya. K. Syrkin and M. Ye. Dyatkina, and also by A. I. Kipriyanov, and in a number of articles published by A. N. Nesmeyanov, R. Kh. Freydlina, B. M. Mikhaylova, Ye. N. Prilezhaeva, M. I. Kabachnik, D. N. Kursanov, and others.
4. Kursanov's report quite correctly points out that heretofore Soviet chemists and physicists criticism of the resonance theory did not expose the basic methodological errors of that theory. Attempts at criticism were neither directed against individual aspects of the resonance theory (V. N. Ufimtsev) or were carried out from a wrong viewpoint (G. V. Chelintsev). Chelintsev's new theory of structure is rather unsuccessful, because his results are not in agreement with contemporary views on the nature of the electron and the observed behavior of organic compounds.

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The Scientific Council resolved that:

1. The fight against idealistic concepts in the field of theory of organic chemistry and work on the development of a contemporary theory of structure and reactivity of organic compounds are to be regarded as important tasks of the Institute of Organic Chemistry. In the future, extensive experimental and theoretical work in that direction will be planned and carried out, in accordance with the demands made by the national economy of the USSR.
2. The fundamental premises of Kursanov's report should be approved and the report published with due consideration to the results of the discussion at the 2, 3, 7 February 1950 meeting of the Scientific Council of the Institute of Organic Chemistry, Academy of Sciences USSR.
3. It is considered necessary that collaborators of the Institute of Organic Chemistry who have used the concept of resonance in past work should correct, in subsequent work, errors which they have made.
4. It is considered necessary to acquaint the Ministry of Higher Education USSR with the report and the discussion which followed the report; also to raise the question of a thorough revision of organic chemistry texts which contain methodological errors (such as the books by Syrkin and Dyatkina and by Kipriyanov), and to point out the undesirability of their continued use without such revisions.
5. A revision of minimum requirements for the Candidate's degree should be recommended, with the view that an accurate reflection of the contemporary status of the theory of structure and reactivity be embodied in courses of study.
6. It is desirable to discuss the question of structural theory in chemical periodicals.

It is the author's belief that the discussion at the Institute of Organic Chemistry has shown that everything is not in the best possible shape on the battlefield of theoretical chemistry and that hostile theories penetrating from the bourgeois world must be combatted with determination.

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